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STRONGLY CORRELATED ELECTRON SYSTEMS & HIGH-T_c SUPERCONDUCTIVITY

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PREFACE

The properties of strongly correlated electrons are topical because of High T_c Superconductivity (HTSC). It is now more than four years after the unexpected discovery of HTSC in cuprates, but its origin and cause remain controversial.

Some theoreticians began to examine BCS and its implications. The others have been looking for different mechanisms of HTSC. They have tried to explain HTSC using small and large bipolarons, anyons, local pairing and quantum size effect. Multiband, extended and negative-U Hubbard models as well as the t–J model have been analyzed using different methods. RVB and flux phases, phase diagrams, magnetic and spectroscopic properties of high T_c materials have been obtained by mean-field, Green functions and cluster approaches to these models. It seems that in HTSC low dimensionality plays an essential role, similarly as in the Quantum Hall Effect. Low dimensional physics is very promising and leads to the anyon superconductivity and discrete T and P symmetry breaking.

The experimentalists have been synthesizing materials and studying the relations among electrical and magnetic properties.

Our aim in organizing this School was to get the two groups together to allow the exchange of ideas, problems and difficulties. The theoreticians listened to discussions of microstructures, spectroscopic evidence of the Fermi edge and the gap anistropy, the experimentalists learned about the phenomenology and miscroscopic theories, the implications of short coherence length, long penetration depth, and so on.

Besides the invited lectures special discussions were designed to explore specific problems that still remain open. There were also one-half hour presentations given by scientists actively working in the fields.

We do hope that the School fulfilled well its tasks. There remained many unresolved questions and we look forward to addressing them in our future School in September 1992.

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A short-range electronic instability in high T_c superconductors

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Abstract

An electronically driven geometrical frustration is suggested in superconductors. Its possible role in superconductive pairing is introduced and discussed in details, as well as a few successful comparison is presented with the experimental results.

Introduction

Bernd T. Matthias a remarkable physicist has summarized in his review paper about the superconductivity in 1971 [1]: "...Although superconductivity at room temperature will always remain a pipedream, temperatures as high as 25-30 K are realistic possibility and will trigger a technological revolution ...". At present we are much over this limit, the scientific world is boiling, but neither the explanation of the new phenomenon nor the technological revolution has not arrived yet. Are we able to explain and to apply these new high-T_c materials (HTSM) or are those only new pipedreams?

The basis for applications lies in the understanding of the phenomenon, in constructing new, stable, well controlled materials with a suitable geometry (e.g. wires, SQUIDS and/or other Josephson-devices, etc.).

In order to understand the superconductivity the BCS theory [2] has been offered. This is an excellent, elegant and powerful explanation of the phenomenon. Unfortunately it has suppressed the thinking dealing with the material-science aspect of the topic. Therefore the BCS is a non-applicable, highly theoretical explanation, unsatisfactory in predicting the actual T_c-s and choosing the definite optimal materials. While the ideas of Fröhlich [3], Labbe [4], Testradi [5], Matthias [6] etc. became unpopular and remained in the shadow of the light of the very general and elegant BCS theory.

Some of the contradictions of the BCS-theory were 'elegantly' forgotten, and only the new high-T_c business has focused the attention on the numerous and serious 'old' enigmas:

- The problem of the non-satisfactory isotope effect (in the 'old', non-ceramic superconductors as well) obviously needs a modification of the pure phonon-mediated pairing. The BCS predicted isotope effect has been observed only for simple metals, neither the transition metals and their alloys nor the new HTSM-s

and other compounds (for example PdH) satisfy the requirements.

- The structure is obviously irrelevant for numerous cases of superconductors. For example the strictly ordered materials having A15 (A_3B, β-W) structure and their amorphous counterparts, (Table I. [7]) show the marginality of the crystalline order alone. On the other hand amorphous Be has a T_c about 350 times higher than its crystalline counterpart, [8]; so the question can be generally asked: what is important, the strict crystalline order (long-range order, LRO) or its loss of leading only to short-range order (SRO) in the material?

- Is the low-dimensionality one of the keys to superconductivity? Answers to this question are very contradictory. For A15 materials the ideas based on one-dimensional (1D) chains were the first clues [9], but it was rigorously shown later that superconductivity is impossible in 1D [10]. Despite this contradiction, the 1D models for A15 superconductors are working well, [11]. To deal with the dimensionality problem for HTSM is more difficult. There were established some low-dimensional models in 1D [12] and 2D [13], but numerous objections are raised against them since the phenomenon is regarded as to be essentially three-dimensional [14], [15]. Some models are working on the basis of mixed dimensionalities, [16]. (Note, the low-dimensional approaches are working satisfactory.)

Is the superconductive pairing established only by phonons,

or are possible other mediators as well? The observations on HTSM-s cannot provide a definite answer.

Even the rule of the 'perversity of nature' is in action: "... For a given class of materials those with the highest T_c-s tend to be less stable and more difficult to make ...", [17]. This presents itself for the HTSM in the sample preparation: if the material has higher and higher T_c the actual sample size has become smaller and smaller, [18].

In consequence of the above enigmas we support the idea that the fundamental phenomenon is a relevant instability (metastability) in superconductivity and especially in HTSM. However to the formulation (in 1972, [19]): "... at the present there are no higher temperatures {'superconductors'} only instabilities..." we can add nowadays: at the present there are numerous higher temperatures {'superconductors'} and various instabilities, but it is a pity that their interdependence has not been clarified yet. In our present paper we suggest a general instability which we regard to be responsible for the enigmas and use it to explain the HTS-phenomenon.

The metastability factors

The metastable structures, or more accurately, the configurationally frozen metastable structures are important in physics. The investigation of materials with compositionally, topologically and/or morphologically metastable is very important.

In the past three four decades, among the new materials produced are glassy metals, highly supersaturated crystalline alloys and new alloys with exceptionally high interface densities.

Much of the early stimulus to activity, directed at the synthesis, study and exploitation of novel metastable structures, especially in metallurgy, demonstrating some metal alloys melt quenched to amorphous solid or "glassy" form. At the quench the system may be "frozen", we will say "configurationally frozen", into one of these intermediate states. Upon annealing this state often evolves into other interesting and useful metastable states. The question of stability of metastable states is still in a phase of rapid development.

The metastability is pertaining to the energy state situated higher than the stable (equilibrium) state and isolated from it by an energy barrier, characterized by an activation energy. The stability questions in most of the cases concentrate on the height and the origin of these barriers. The most important factors creating this barrier from the material-science point of view are:

1. Chemical factors, (Hume-Rothery [20], Pauling [21], Pearson [22], etc.):
   - chemical bonds,
   - electrochemical differences,
   - electronegativity differences, etc.
2. Geometrical factors, (Hume-Rothery [23], Laves [24], Frank and Kasper [25], etc.):
   - size factors,
   - tendency to proper space-filling, etc.
3. Electronic factors, (Hume-Rothery [23], Jones [26], Mott [27], etc.):
   - electronic band effects,
   - collective quantum-effects, etc.

All these factors are connected with electronic bonds and bands, and all are different manifestations of the electronic properties of solids. No chemical and geometrical effects are understandable without the essential electronic effects, which are of course a-priori responsible for metallic and other type of bonds.

One of the central ideas of our present paper is that the metastable states in solids are stabilized in a small energy range by their electronic (band) structure, through the effects that the band structure is accommodated with lower energy in metastable phases than in their stable counterpart, [28], (Fig. 1.).

Structural properties

The topologically close-packed structures were intensively studied by Laves [24] and Frank & Kasper [25]. It was pointed out, that many complex intermetallic compounds can be understood as being determined by the geometrical conditions of sphere packing. The space packing requires tetrahedral microarrangements and in general the energetics of the packing favors the structures with

triangular faces, and tetrahedral cells.

The packing of an individual cluster consisting of uniform spheres prefers the coordination number (CN) of 12. Three types of the close-packed coordination with CN = 12 are existing: the face-centered cubic (FCC), the hexagonal close-packed (HCP) and the icosahedral close-packed (ICP). The FCC and HCP are space-filling structures, their periodic repetition is filling the space properly. These two structures appear very commonly in the crystalline materials, having well defined LRO with dense packing. The ICP structure however is very peculiar: it cannot fill the space properly, but leads to the densest packing, [25]. This structure consists of twenty slightly distorted regular tetrahedra (their height is reduced by a factor of 0.925) sharing one vertex, the center of the icosahedron. This tight tetrahedral packing is the origin of the preference of the icosahedral arrangement, which -as calculated by a simple potential-well approximation [29],- is the energetically most stable clustering, using realistic soft, deformable spheres for packing.

Indeed in clustering processes the short range order (SRO) is striving to the icosahedral formation under certain conditions. This process was experimentally observed in various liquids and amorphous solids, [30]; in the formation of extremely small clusters, [31]; moreover even in the austenitic stainless steel [32]. The icosahedral coordination is existing in metallic crystals [33] and in non-metallic compounds [34] and was as well observed in metal-carbonyl clusters [35] playing an important role

in catalysis. The most interesting fact in this point of view is the cluster formation in cluster-beams, showing a preference for some definite clusters (the number of atoms involved in these clusters give the so called 'magic numbers'), which can be described well by icosahedral arrangements, [36]; so the small clusters of atoms tend to form icosahedral clusters.

To study the local structures the concept of the so called Voronoi polyhedron [37] can be introduced in general. These polyhedra represent the first coordination shells of every atom by a convex polyhedron formed by the perpendicular bisecting planes of each atomic bond, [38] (in crystalline materials this construction is called the Wigner-Seitz cell). In filling the space by spheres the five-fold symmetry is frequently preferred in the Voronoi polyhedra, seeking to the ICP arrangement, [39]. Nevertheless the short range local preference of the icosahedral order cannot agree with the global long-range requirements. The icosahedra (as well the dodecahedra as their dual [40] and simultaneously as its Voronoi-polyhedra) have not perfect tessellation in the Euclidean-space due to their five-fold symmetry [41].

Consequently the closest cluster packing (ICP) creates a funny situation: in the point of view of space filling the SRO prefers the ICP arrangement, while the LRO requirements favor the different structure because by a periodic repetition of only icosahedra the proper space filling does not exist. In this meaning the SRO and LRO requirements are contradictory. The actual

stability of an arrangement has been determined by the balance of the contradictory tendencies in long- and short-range potentials .

For the long range potential term there are various approximations. The simplest and so the most popular is the jellium model, widely applied in the theory of metallic clusters, [42]. The shell approximation with the spherical jellium model describes some observations of cluster creation in the alkali metals well, [42] but with magic numbers (MN) different from the case when the material is modeled by the Lennard-Jones potential. On the other hand some experimental facts, (for example some metals having MN = 13) have no explanation in this picture. Indeed with a spherically averaged pseudopotential, (SAPS [43]) or in the case of an other mezoscopic potential, (an average Madelung energy proposed by Manninen, [44]), which are effective only in the mezoscopic range, the results obtained are closer to the experiments. The 'geometric effect' (the local energy requirement) leads to a special stability with clusters of five-fold symmetry, first of all for clusters containing 13 atoms, [25]. The vacancy formation energy for different clusters is the highest for the icosahedral clustering, but the cluster arrangement is gradually disappearing during growth, (as the influence of the long-range term is growing), [43]. On the basis of these calculations [43] it is clear, that the alkali metals and the molten phases may overemphasize the spherical (jellium) structure, suppressing the role of the packing geometry, while the non-alkali metals have clustering effects for which the jellium long range average is not satisfying. In general the jellium-like (drop) clustering is preferred by the good metallic materials, [45] while the materials with large electron effective mass form more likely ICP arrangement, which is generally described by the Lennard-Jones potential, [29].

The cluster of the ICP closest packing cluster can be well enlarged by a so called disclination procedure [46] into a higher coordination arrangement. This procedure creates different Frank-Kasper polyhedra with CN = 14,15,16. It is well established, that these Frank-Kasper phases give the topologically ideal close-packing in comparison to any other packing constructions, [25]. These phases have in average five-fold faces [47], which emphasizes the crucial role of the SRO in close packing.

Geometrical frustration

The apparent contradiction of the space-filling in short range (the highest cluster densities have five-fold symmetries) and in long range (for the proper translational tessellation the five-fold symmetry is definitely prohibited) can be solved in different ways.

Let us consider the effect of the five-fold symmetry in a simple two-dimensional lattice containing regular pentagons translationally arranged in a sheet. The plain sheet cannot be covered properly by these pentagons, in addition an other polygon (rhombus) has to be applied for tailing, (Fig.2). This is one of the solutions, when the short range five-fold requirement is

satisfied and the plain is filled . In this case not all the clusters are in the preferred pentagonal arrangement, the system contains rhombuses far from the optimum pentagon. This frozen-in solution solves the SRO ↔ LRO contradiction in the way of partially satisfying both of the requirements as well. Of course the overlap of pentagons (Fig.3.) is also harmonizing with the LRO space filling but the first coordination circles are not pentagonal, contradicting to the initial conditions.

The other possible arrangement is to deform the regular pentagons to non-regular polygonal forms (Fig.4.) where the LRO can be easily satisfied. These deformations are frozen-in and so the optimum SRO is heavily damaged in each micro-arrangement. If these deformations are not frozen in, the particles in the fence chains are frustrated (soft bonding case). These atoms have no fixed optimum site, and fluctuate on the given linear chain satisfying both the SRO and LRO requirements in a time-average of their motion, (Fig. 4/*b*. and Fig.5.). Consequently the SRO ↔ LRO problem is soluble by a non-frozen, dynamic arrangement: the rigid puckered chains and soft, fluctuating fence chains are altering (Fig.5.). If this arrangement somehow freezes, then both of the long- and short-range requirements are broken.

We note, that the tessellation of regular pentagons can be arranged in different ways (for example Fig.6.) where the solutions will be different than the above described, but the basic idea is applicable in every cases.

One of the serious questions is the existence of a continuous transformation of the long-range ordered arrangements to the short-range favored clustering. Without this transformation the balance of the SRO and LRO is not tunable, the frustration picture is not realistic. The continuous transformation from a rectangular square lattice to the tailing for quasicrystalline tessellation is solved [48], by the tilting of the lattice units. A continuous tessellation by pentagons can be also achieved from a square lattice, introducing a special deformation at the appropriate places, (Fig. 7.). Shrinkage and expansion of the original square-network must deform it in to the regular pentagonal tessellation like in Fig.2. This effect corresponds to the special projection of the curved sheet into a plain 2D arrangement.

Having learned the processes in 2D, we turn now to the 3D packing problem. The contradiction of the optimal structural energy in local and global scales derives from that by the locally most stable icosahedral clustering is unable alone for proper tessellation in three-dimensional Euclidean-space. If the short range interactions are strong enough to influence the general energy balance, the structure has to be frustrated. The competition of the two antagonistic mechanisms can produce indeed a set of similar structures and equilibria. The properly space-filling FCC or HCP clusters can deform spontaneously to the icosahedron [49] creating the most dense packing in a cluster, so the possibility of the solution of LRO ↔ SRO contradiction by the same dynamic picture (as was described in 2D) is existing. A slight deformation can transform the FCC to ICP and vice versa

As a matter of fact the FS-JZ interaction determines the stability in partially and/or totally disordered (LRO is lost) systems, [28], [66]. The homogeneous and isotropic disorder with SRO and MRO, makes possible to define a periodically continued neighborhood [67] and quasi-Bloch states [68] in one-electron approximation. For such materials a sphere-like JZ has been measured by diffraction methods [69], and a nearly-free electronic behavior has been observed [70] as well. In consequence one of the most powerful ideas for stabilization of amorphous metals (the Nagel-Tauc theory, [71]) is based on FS-JZ interaction, [69].

For the electronic stability the perfect nesting of FS in JZ is the optimal case, the increase of the electron-number due to the energy-gap at the FS, requires a large energy to surmount the gap. To create this stable nesting the JZ should have polyhedra close to the sphere [28], having a large number of faces in uniform distance from the center of the zone. The FCC JZ has 8 faces for the first touching, while the JZ of ICP (which is icosahedron as well [55]) has 20. Consequently the icosahedral arrangement is the most stable taking into consideration the JZ-FS interaction, (and of course the appropriate number of electrons needed to create the nesting of FS) [28].

The electronic structure calculations show the stability of different LRO symmetries [72]. Two well defined electronic concentrations has been found where the material has not any preferred LRO (Fig.11.). In consequence of the non-definite LRO, these compositions have to have a strong SRO effect, seeking to the icosahedral or other Frank-Kasper coordination, creating optimal SRO for stable clustering. This SRO arranges a special MRO effective in a few coordination shells [73].

Structural aspects of HTSM

The group of superconductive material is very wide: elements, binary-, ternary- and more complicated alloys and compounds. There is no curiosity found either in their conductive behavior, the structure in the normal state, or any specific property. This is the reason, why is it so difficult to predict the superconductive T_c or other relevant and important superconductive characteristics of the materials involved. Their almost common feature is only their lattice instability, which is consequently observed in many important cases. A drastic phonon softening is predominating leading to a martensitic-like transformation accompanied by a substantial enhancement of T_c at larger instabilities. The correlation of T_c on martensitic phase transition and lattice instabilities was shown among others by Testradi [5] and Phillips [74].

Another general structural observation is that in many cases the superconductive materials have Frank-Kasper coordinations, very often with CN = 12. A clear example is the A15-structure of A_3B compounds, where the A-type atoms (atoms in chains) form icosahedra, while B-type sites are arranged in the other Frank-Kasper clustering with CN = 14 [75]. Furthermore it is

(Fig.8.), [50]. The LRO preferred FCC (Fig. 9/a.) can be continuously deformed into a tessellation seeking to the ICP clustering (Fig. 9/b.) and finally we get a tessellation by regular icosahedra (Fig. 9/c.). This process is more spectacular on the corresponding Voronoi polyhedra, where the continuous tilted deformation of the polyhedra from the FCC Wigner-Seitz cell (Fig.10/a.) through a transition phase (Fig.10/b.) to the regular dodecahedron is clearly seen, (Fig.10/c.). Consequently the apparent contradiction of the packing problem in long- and short-range is solvable by the same dynamic way as was in 2D, if we are near to an instability, balancing between the preferable SRO and contradictory LRO clustering.

In actual materials the local (SRO) and global (LRO) energy requirements compete with each other for evolving the structure observed. It is supposed, that their balance has a central role in the formation of the actual phase, emphasizing the crucial role of the medium range order (MRO) in the mezoscopic region. The balance of SRO $\leftrightarrow$ LRO interaction (instability),- we suggest,- can be tuned by MRO of the solids. To examine the MRO let us consider a system seeking to icosahedral clustering with non-interacting spheres. Switching on an attractive potential between them, this tendency is remaining, [49], a strong potential minimum of the arrangements with tetrahedral cells and triangular faces [51] is observable. For the description of the atomic interactions the Lennard-Jones potential is frequently used, which strongly stabilizes the ICP structure through a few (about 8-11) coordination shells [52]. Moreover the number of atoms which are involved in a volume stabilized by icosahedral symmetry is relatively large, ranging between 10^5-10^7 [53]. These problems are giving rise to heated discussion in the literature just at present, [54]. The optimal dynamic harmony of local and long-range stabilities and its possible freezing depends on the range of interactions. The strong short-range forces without the medium effects in mezoscopic ranges cannot form a dynamic frustration because any arrangement would be frozen-in all the time. The coupled first coordination shells (local order of clusters) can be frustrated in long range only by active medium range forces.

We note, that the contradictory SRO $\leftrightarrow$ LRO conditions can be harmonized statically as well in the 2D picture. If we pick-up the rhombuses from the tessellation in Fig.2. and close the leakages in the space, the sheet becomes curved, the problem turning into the curved 2D representation. Twelve pentagons form a regular dodecahedron, where the pentagons are filling the 2D surfaces of the regular dodecahedra in 3D, without any difficulties. Forming these dodecahedra by each twelve pentagons, the 3D space will be filled up by dodecahedra, but not properly. With further cutting out the interpolyhedral spaces between dodecahedra, (shrinking in the space) the problem becomes one of the curved 3D space, giving a polytope solution [55], where the dodecahedra can fill the space of higher than 3 dimension, properly [55]. This is a static solution in the more than three dimensions. In 3D-cases the curved-space description has been introduced for the amorphous and quasicrystalline structures, [30],[56],[57], too. Considering the relaxation effects [58] in the realistic models, the number of

observed that the superconductivity of these alloys is highly sensitive to the impurities on A-sites while are much less influenced by B-type atomic sites, [76]. In the amorphous alloys the Frank-Kasper coordination with CN = 12 (icosahedral) is quite common [39], so a strong short-range effect has to be expected in these materials.

The Frank-Kasper phases and especially the CN = 12 coordination is also common in the HTS-materials too. The twelvefold coordination is arranged generally as three perpendicularly twisted squares, (Fig. 12) being very much similar to the arrangement for easy FCC ⟷ ICP transformation, (Fig.8.). This arrangement could be involved in a frustration as shown for example in Fig. 13.

The special structural transitions observed (orthorhombic ⟷ tetragonal [77], rearrangement of oxygen-vacancies [78] etc.) are generally connected with the rearrangement on the clusters with CN = 12. According to a careful Voronoi-analysis in HTSM-s the average symmetry of polyhedral faces is characteristically close to five, [79]. The marginality of the sheet or chain structure is clearly shown by the existence of the metallic but not superconducting La-Ba-Cu-O and La-Sr-Cu-O systems [80], in which there is no correlation between the special structures and the superconductive behaviours.

The selectivity on the replacement of different atomic clusters is very similar in HTSM as in A15: for example

$Y_1Ba_2Cu_3O_{7-\delta}$ is much less sensitive for its Y-sites (CN = 16) than for its Cu-sites (CN = 12).

Electronic aspects of HTSM

The preference of SRO against LRO, - as we mentioned above, - is trivial in some special definite electronic concentrations. The effect of FS - JZ interaction on superconductivity is well substantiated: enhancement of T_c arises from the FS interaction with the JZ, [81]. It is well established and supported by experiments, that relative maxima in T_c are to be expected in structures in which the FS touches a large number of JZ boundaries; causing an infinite, logarithmic van-Hove anomaly [82] corresponding to energies when the surface of constant energy just touches the JZ boundary. The effect of van Hove singularity is also one of the popular explanations for the HTSM phenomenon, [83].

The data of high-resolution angle resolved photoemission spectroscopy and positron-annihilation measurements are consistent with the existence of a Fermi surface. The states near the FS are mixed O 2p and Cu 3d, and the DOS has a sharp Fermi edge. As a matter of fact the changes measured at the Fermi-energy [84] allow us to suppose the suggested interaction between FS and JZ, observing a sharper Fermi-edge in the superconducting materials, as in their normal counterparts.

The electronic concentration has a strong effect on the T_c of

superconductors, as was empirically found by Matthias, (so called Matthias rule, [85]). Furthermore we observed [86] a striking correlation of the strong SRO preference with maxima of T_c versus the electronic concentration both for A15 and for amorphous superconductors. The new high T_c ceramics also fit well in this picture, (Fig.14.).

The parent materials of all the HTSM materials (such as La_2CuO_4, $BaBiO_3$, $Y_1Ba_2Cu_3O_6$, etc.) are nonmetals. In their electronic structure a completely filled valence band is followed by a forbidden gap and an empty conduction band. The FS is nesting tightly in JZ, which is a stable position for the electronic band structure because to turn this nesting state into a metallic one by electron doping an additional energy is required to surmount the energy gap around FS. The total nesting is tuned away (T- T^*- and T'-phases) by free charge-carrier doping (electrons or holes), [87]. The materials have become conductive while the electronic structure in general is not so far from the stable non-metallic case from where the system was only slightly tuned away. Seeking to form a stable electronic situation the SRO clustering seeks to reach an arrangement which is optimal for the nesting in k-space. This nesting can be satisfied by 'magic' clustering [36] in short range [39] in the same manner as in the free clustering. Creating jellium-like 'drops' to minimize the electronic energy satisfies both the LRO and SRO requirements, because these drops are of the symmetries which have not five-fold arrangements, so can fill the space properly.

A special problem arises, if the free-charge carriers are much less than needed for the jellium, no effective long-range interactions are existing, consequently the icosahedral 'magic' numbers are preferable. The icosahedral ordering creates proper nesting of FS in JZ, which is an electronically stable arrangement.

Frustration and pairing in HTSM

The parent materials with full nesting of FS in JZ are non-metallic. (The FS nesting in 2D is schematically given in Fig.15/a.) the parent materials are homogeneous both in SRO and LRO having definitely the same nesting (electronically stable) condition everywhere. Adding a few free charge carriers to the system, the nesting is suppressed (Fig.15/b.); and the system becomes conductive, having the same FS - JZ interaction in each cluster. The only slight tuning away from nesting gives possibility to the system to seek to the electronically more stable nesting situation. To create the optimal SRO, (which is most stable) the fluctuations become collective and coherent in short and mezoscopic ranges. The electronic structure driven such collectivity prefers the relevant icosahedral Frank-Kasper clustering.

On the other hand, the charges collected in this way from short range to a nesting situation will be missing from the neighborhood and the dense SRO (or the nesting in k-space) becomes impossible in the near vicinity. This enhances the total energy

for the region around the locally stable cluster, so in average the energy-minimization of the system is not as effective as could be without the LRO requirements. The solution of this problem can be a dynamic frustration which was introduced before.

When the LRO and SRO requirements are balanced in the same manner as we described above, a geometrical frustration takes place in the material due to the incompatibility of the global and local tendencies. The momentarily optimal SRO cannot be frozen in, because its neighborhood becomes more instable by the stabilization of the given cluster. The solution is a breathing like dynamics which can mediate the pairing requested for the superconductivity in BCS meaning.

The pairing,- the attractive interaction between a couple of electrons,- has in its essence very similar mechanism as in BCS. The pairing is based on the instability due to the vicinity of FS-nesting. The effective mass of the individual electrons is high in this region [88], leading to a small kinetic energy. For this reason the next electron can be easily captured into a potential-well created by the stable nesting. This effective pairing mechanism becomes anomalously large at the near vicinity of nesting, which is more enhanced in the case of Frank-Kasper clustering because of the JZ is almost spherical due to the closest packing. This pairing mechanism corresponds to the BCS with the only difference, that instead of the (virtual) phonons a non-harmonic instability mediates the coupling by the (virtual) cluster breathing. The direct comparison of the DW measurements

made on HTSM Y-Ba-Cu-O and Y_2O_3 both on 80 K show a larger DW for HTSM as for Y_2O_3, [89], and it was pointed out [89] that a structural disorder must be also present.

The mezoscopic structures observed in HTSM-s strongly support our ideas. The mezoscopic wavelength of the superstructures for HTSM-s is eight atomic distances [74], which agrees with the effective length of the icosahedral forces (8 shells) calculated by Lennard-Jones potential. The icosahedral-like mezoscopic effects are also supported by the observation that the diffraction patterns are compatible with the four-dimensional space groups Bb2b(1β)(1-11), Bbmb(1β0)(1-11), Bb(0$\beta\gamma$)(1) and B2/b(0$\beta\gamma$)(-11) [90], in which -according to our suggestion- the intrinsic curvature of the icosahedral clustering [91] appears. The measured characteristic optical transitions [92] involve electrons in the Cu-O chains, and furthermore the observed rigidity of the yttrium neighborhood [89], and 'soft'-chains in the Cu-cluster-neighborhood (between the Ba contained layers) [89],[93] in the $Y_1Ba_2Cu_3O_{7-z}$ model system, and similar ones in the thallium-compounds [94], are supporting the icosahedral seeking.

There are observations about the anisotropic oxygen displacements which are strongly coupled to the origin of the high-T_c superconductivity [95]. Furthermore the strong anharmonicity of the oxygen vibrations is also well established theoretically [96],[97].

These experimental facts allow to suggest the existence of

the dynamic frustration in HTSM-s, where the coherent and collective fluctuations [98] are due to the relatively large thermal fluctuations in the (CN = 12) clusters, giving opportunity to the optimal clustering in the system.

Fluctuations

The temperature dependence of the Debye-Waller (DW) factors (measured by neutron diffraction in the $Y_1Ba_2Cu_3O_{7-z}$ system [99]) is not the same for all of the ions involved. In contrast to the yttrium DW, the relative thermal fluctuations of the first coordination cluster of Cu are very peculiar in the chains. Let us compare the DW-s of different atoms! Their temperature-dependence is not the same, the DW of the Cu-neighborhood changes with the temperature more strongly than of the Y-neighborhood. We introduced the relative DW-s, (DW_r = DW/DW_Y). DW_r-s are enhanced below T_c(= 92.5 K) ($\Delta T/T_c$ = -0.23) compared to the temperatures above ($\Delta T/T_c$ = 0.34) in the same orthorhombic phase (Fig.16.). In the superconductive state a remarkable relative enhancement of thermal fluctuations can be observed in the region of the Cu coordination sphere. The temperature dependence of the DW for the Cu-O bond indicate that the Y-Ba-Cu-O below T_c is more disordered as expected, [89], [100]. If we compare the relative Debye-Waller-factors of the samples which were irradiated by different flux of fast neutrons, [101], we can see, that they decrease parallelly with T_c (Fig.17.). In the case of $La_{1.85}Sr_{0.15}CuO_4$ a similar but much smaller effect was measured [102] (Fig.18.). An anomalously large

DW was observed for oxygen atoms (involved in frustration as we suggest) in $Tl_2Ba_2CaCu_2O_8$ too, [94].

Fig.19. shows the DW-factors of Bi-Sr-Ca-Cu-O at room temperature for different compositions [103]. The DW-factors of Bi, Sr and O(1) atoms increase with T_c while the behavior is opposite for Ca and O(2). This shows a tendency for a sandwich-system in which the relatively rigid and the relatively soft (large thermal fluctuations) layers alternate. This is optimal for the dynamic-frustration suggested before. The correlated displacements were observed experimentally in the A-15 phase of Nb_3Ge [104] and in other A-15 superconductors [105] too.

The relative DW-factors are in correlation with the measured resistivity anisotropies [106], which increase about 2-3 times at low temperatures. In consequence of the increased anisotropy, the cluster effects are well emphasized at low temperatures. A strong 3D fluctuation behavior has also suggested [107] on an other basis.

Furthermore the fluctuations of the order-parameter are large too, so no mean-field range should be observable in the higher T_c (Bi and Tl oxides) materials, [108]. The HTSM-s must be considered as superconductively inhomogeneous on the scale of the unit cell, [108]. It is shown [109] that the mechanism of doping provides a coupling of lattice vibration and charge-transfer vibration modes. An anharmonic motion of O-ions in the fence chains of $Y_1Ba_2Cu_3O_{7-\delta}$ and in the (La,Sr)-O(2) plane for

$La_{2-x}Sr_xCuO_4$, (so out of the CuO_2 planes [110]), is in support of our suggestion. The anharmonic character of the chain vibrations may be the essence of the cluster-anharmonicity as well.

Based on a local instability, short-living ($\tau \cong 10^{-13}$–10^{-12}) and large energy fluctuations were suggested [111], and applied in the kinetic theory of melting [112]. These instabilities exist in both the high-T_c and low-T_c superconductors, [112]. The coherence of the fluctuations has been suggested by us above. So a collective glide of a stable arrangement is possible through the material.

The concept of elementary excitations has been made use of in the case of frustration, [113] similarly to the Bragg-condition in crystalline material, a spherical JZ can be assumed in amorphous materials with radius $2\pi/d$, (where d is the average distance of atoms). A soft-mode appears near $k = 2\pi/d$ in such solids where the frustration is in action. This is similar to the quasiparticle 'solidon' which was introduced in He_4 [114]. According to our suggestion [98],[115], there is a collective excitation mediating for the electron pairing in high-T_c-materials, in consequence of the frustration. The soft mode predicted near $k = 2\pi/d$ [113] acts in the vicinity of the JZ-FS interaction emphasizing repeatedly the role of the electronic structure.

We are convinced [115] that the dynamic frustration effect is responsible for the new HTSM-phenomenon. The displacements are

caused by the breathing [115], in good agreement with dynamic Jahn-Teller assumptions [116], and with other vibronic [117] and collective-dipole-mode oscillations [118].

The oxygen displacements breaking the symmetry in superconductive oxides [119] have anomalous temperature dependence. Our explanation of the thermal displacements is that they are only apparently uncorrelated. Correlation is coming in action in the first coordination shells, driven by SRO and independently with the LRO requirements. The break of the symmetry of LRO structure obviously is one of the special features of the HTSM in connection with the essential mechanism of the electron pairing, [119]. We mention that a coupling based on a short range deformation has been suggested for the ferromagnetic clustering [120], which regarding the SRO-coupling is similar to our considerations.

The periodicity which is expected from the cluster-mediated pairing has been observed in superlattice structures of HTSM, [121] [90]. There have been emphasized [90], that the observed modulation can be described by the four-dimensional space group [90] that is consistent with the proposal of icosahedral seeking, since it can be described most clearly in the curved 3D space too [61]. This modulation (mezoscopic structure) is stabilized by the MRO. A superstructural periodicity with a wavelength of 8–11 atomic distances was observed [121], in agreement with the calculations by Lennard-Jones potential for ICP structures, [52], and with observations pointing out the relevance of icosahedral

seeking in HTSM. On the other hand the mezoscopic idea is widely applied for explaining the quantum size effect (QSE) of high temperature superconductive phenomenon [122].

Further support of icosahedral idea is the similarity of the PIM arrangement with superconductivity which is obvious in the light of the phenomenological Ginzburg-Landau description, [123]. Introducing a certain order parameter in this randomly disordered material (in meaning of LRO) [30], an uniformly frustrated Ginzburg-Landau model of statistical mechanics can be constructed, clearing up the formal analogy between the Ginzburg-Landau theory of superconductivity and the gauge field theory of predominantly icosahedral materials (PIM) [15],[60]. The disclination network in PIM corresponds to the Abrikosov flux lattice while the disclination flux exclusion is the analogy of the Meissner-effect in superconductors of type II. So we may regard the enhanced short-range icosahedral order at the relaxation process as expelled magnetic flux lines. In this way the superconductor-normal phase transition is similar to a phase transition from amorphous state (dominating SRO) to the dominating LRO structure, (crystallization).

Isotope effect

Although a consequence of the BCS-theory is the isotope effect. A strict isotope effect however was not found at all in most of the 'old', metallic superconductors [124]. Furthermore a lot of T_c-s are higher than 40 K which is hard to interpret by the

pure phononic mechanisms, [125].

If the pairing is mediated by clusters than (on the same reason as for the phonons in BCS), the cluster mass has to be responsible for the change of the superconductive temperature. It is well known in BCS that the critical temperature (T_c) depends on the isotope mass (M) in the following form:

$$T_c \propto M^{\alpha} \qquad (1)$$

where α is -1/2 in the ideal case. We showed in our previous paper that [115] this isotope effect is mostly nonexistent including the HTSM too. The comprehensive figures on isotope effects [115] have been redrawn, (Fig. 20. and Fig. 21.) for clarity. The lower than expected values of α can be explained by the cluster effect, which means, that the larger cluster mass must appear in Eq.(1). [115]. The ΔT_c in these cases is almost independent of the T_c, (Fig. 21/a) which can be explained by the small relative change of cluster masses for the change of the oxygen isotopes, the exponents are not constant, but depend on T_c (Fig. 21/b.).

Reevaluating a set of the measurements [126] from the point of view of clusters we can calculate the relevant masses. For example in the $Y_1Ba_2Cu_3O_{7-\delta}$-structure the frustrated cluster is a layer between the Ba-containing layers [115] (Fig. 12.and Fig. 13.)

Thus the cluster mass can be calculated using the sum of

atomic masses of the $Ba_{2-z-y}La_yCa_zCu_1O_{2+x}$ compounds [126] on the assumption that the formula of this ceramic is actually $Y_{1-z}La_zBa_{2-z-y}La_yCa_zCu_3O_{6+x}$, assuming that the La atoms prefer the Y sites against the Ba sites because of their chemical similarity. The T_c dependence versus the inverse square-root of the cluster-mass is presented in Fig.22., where the points fall on distinct straight lines according to the parameter z, showing the predicted linear dependence. The fitting parameters (r) of the linear regression are collected in Table II. The cluster mass $M_{cluster} \cong 390$ can be extrapolated when $T_c=0$ corresponding to the composition of $La_2Cu_1O_{2+x}$, which is close to the relevant inner cluster of the well known, La_2CuO_4 insulating parent-compound. This correspondence however is not yet entirely clear posing a new challenge. Fixing the relatively rigid bonds [89],[127] the frustration process is similar for different masses of the cluster as have been shown in two dimension (Fig. 5.). By analysing other data, [126], [128] the mass dependence of T_c is linear, Fig. 23. [126], Fig.24. [128].

This special behaviour of clusters has been observed in the thin superconductive layers in dependence of their thickness. If it is assumed that the volume of the cluster is proportional to the mass and the thin layers are homogeneous, the T_c versus $(1/d)^{\alpha'}$ graph must be linear with an α' about 1.5. From the analysis of the measurements of Haviland et al [129], the best fit for Bi-layers is $\alpha'= 1.49$ while for Pb $\alpha'= 1.23$, (see Fig.25). This effect can be observed in Nb-films ([130], too, Table III.).

The cluster-type isotope effect is well supported by a very

recent calculation for layered HTSM superlattices, [16]. The calculation is very general, not using any definite pairing mechanism for the high T_c phenomenon. T_c is given for N of HTSM layers divided by insulators:

$$T_c = 4082 \exp\left\{\frac{-1}{0.188 + 0.084 \cos[\pi/(N+1)]}\right\}$$

in good agreement (Fig. 26.) with the

$$T_c \propto M^{-0.5}$$

suggestion and with the measurements as well.

Special effects

The transport properties depend sharply on the percolation behavior of perfect superconductive regions. At a given temperature the expression

$$R(d) = R(0)(d-d_c)^{-s}$$

was proposed for the resistivity [131],where R(d) is the resistivity of the layer with thickness d, R(0) is constant, exponent 's' is theoretically 1.3 and 0.75 [131] for two- and three-dimensional percolations, respectively; and d_c is the critical thickness at the percolation threshold, found to be temperature independent, [132]. The critical thicknesses were found to be pretty small, for example in Bi $d_c=0.408$ and in Pb

d_c=0.186 nm, [129]. Special superconductor-insulato transitions were observed in many cases [129],[133] for increasing film-thickness, but in nominally homogeneous thin films [131] no evidence for the local granular superconductivity was found at low temperatures. For high temperatures the quantum-resistance of pairs ($R_c = h/4e^2$) divides the thin films into two categories [134]: one of them becomes superconductive, the other insulating at low temperatures. Consequently there is an obvious bifurcation between the normal states of the insulating and superconducting films with threshold of the universal sheet resistance (R_c), [134]. This critical threshold R_c is independent of any details of the actual sample as its size, disorder, granular structure, etc.

The physical background has been explained [134] as follows: Let us consider the Anderson localization [135]. When the localization length (L(E)) for an electron with energy E is significantly smaller than the average size of the Cooper pairs required for superconductivity, the Cooper pairs cannot form, being only localized electrons in the system. Therefore the system remains in the insulating state even at temperature T=0. In the opposite case L(E) is greater than the average size of the Cooper pair consequently the superconductive state can be established. This leads to introduction of a critical localization length (L_c) which corresponds to the average size of the Cooper pairs. If L(E) is greatest at the Fermi energy E_F, the L_c and $L(E_F)$ values are relevant in the point of view of superconductivity at temperature T=0. On the condition $L(E_F)<L_c$ the system is insulating, and for the case $L(E_F)>L_c$ is superconductive. By increasing E_F when

$L(E_F)<L_c$, the localization length L(E) increases, and the material turns from the isolating state to superconductive. This is the case when $L(E_F)=L_c$, creating the critical threshold (R_c) in sheet resistance introduced before at critical $E_F = E_c$.

In the superconductive materials the topological frustration can change E_c in the local arrangements, giving possibility to turn the material into the insulating state, considering the sandwich-type structure of the HTSM-systems. There is a sensitive balance of charge from cluster to cluster behaving as driving force of the frustration in the materials, [115]. This charge frustration can be responsible for the behavior of the transport properties, too, what is an other clustering effect to promote the discussed frustration [115]. It supposes a percolation-like connection between the clusters, giving a possibility for transport superconductivity. In this point of view are interesting the observed
differences of the isotope effects which were measured by the transport and magnetic properties of the same sample, [136]. In every case the changes of T_c due to the substitution of oxygen isotope are larger (up to 60%) in the magnetic measurements than in the transport one. That agrees with transport superconductivity to involve larger, more 'open' clusters. Similar percolation induced conductivity has been suggested by others [137], but on other grounds.

Our idea is supported by the metal-insulator transition measured in YBCO-system in dependence of the oxygen content,

[138]. There is a frustration threshold in the oxygen content at about x = 6.37, measured by transport properties in the $Y_1Ba_2Cu_3O_x$ system.

Conclusion

A dynamic frustration effect controlled by the electronic structure has been suggested to explain the superconductivity. The topological frustration is realized by coherent anbd collective thermal fluctuations in a local cluster-range of the crystal. This type of fluctuations is tunable by the electron or hole doping. According our suggesion, a special clustering in mezoscopic range is responsible for the high T_c superconductivity. The anomalous isotope-effect as well as the special material-dependent behaviour of the high T_c phenomenon has been explained by this picture. A cluster-mass dependence of T_c has been found which is in many aspects similar to the well known isotope effect. A check-list (after Geballe, [139]) is presented (Table IV.) for comparison of basic experimental observations with their possible consequences and their relation to our present explanations.

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Table I. Comparison of T_c-s of some selected A_3B compounds.

Material	structure	
	A 15	Amorphous
	transition temperatures (K)	
Nb_3Ge	23	4
Nb_3Sn	18	3
V_3Si	17	< 1.5
Mo_3Ge	1.5	7.2
Mo_3Si	1.4	7.5

Table II. Linear regression standard deviations (r) and T_c versus $M^{-0.5}$ for a set of $Y_{1-z}La_zBa_{2-z-y}La_yCa_zCu_3O_{6+x}$ superconductors.

$Y_{1-z}La_zBa_{2-z-y}La_yCa_zCu_3O_{6+x}$		
z	r	Value at T_c=0
0	0.98802	0.050575
0.1	0.8946	0.050893
0.2	0.5834	0.050919
0.3	0.4350	0.052568
0.4	0.5033	0.052568
0.5	0.2618	0.013691

Table III. Linear regression standard deviations (r) of Nb thin films based on the clustering assumption.

Assuption for α	r
1	0.9811
1.5	0.9902

Table IV. Check-list [139] of experimental observations, their consequences and relations to our present explanations.

EMPIRICAL OBSERVATIONS	POSSIBLE CONCLUSIONS	Status to our present suggestion
Cu-O layers and chains appear in all HTSM, but there are metallic and not SC compounds	Layers and/or chains are important but not necessary	OK
Magnetic RE substitution do not affect T_c	RE layers are not relevant to SC	OK
T_c=30K in non-cuprate ceramic HTSM	the SC mechanism is similar to cuprates?	OK
jump in thermal conductivity at T_c	strong electron-phonon coupling	OK
Incommensurate CDW in BSCO	A Fermi Surface instability is involved	OK
No BCS isotope effect	non-phonon mechanism	OK
Parent materials are insulators	strong correlation effects?	OK
ρ(300K) > 250$\mu\Omega$cm in YBCO	low carrier density large effective mass	OK
Hall number decreases with T	carrier localization	OK
The magnetic susceptibility is similar in SC LSCO and YBCO, but also in non-SC $La_2SrCu_2O_{6.2}$	the magnetic susceptibility is unrelated to SC	OK

Relaxation rate proportional to T_c and ns in μSR	all carriers participate in SC	OK
perfect reflectance for $\hbar\omega < 250-400\ cm^{-1}$ at $T<T_c$	gap opens below T_c	OK
Strongly damped free carrier absorbtion in optical spectroscopies	charge carriers very strongly scattered	OK
the optical absorbtion is T-dependent at low-frequencies	interaction with low-energy excitations	OK
interband transition edge ($\approx$ 2.1 eV) shifts with T	strong electron-phonon coupling	OK
340 cm^{-1} phonon softens at T_c (Raman)	gap > 340 cm^{-1}	OK
strong electronic background up to 1 eV (Raman)	continuum of localized electronic states	OK
Fano resonance of some phonons with the electronic background (Raman)	strong electron-phonon interaction for those optical phonons	OK
Pseudogap $2\Delta \cong 4-7\ kT_c$ (Raman)	strong coupling?	OK
plasma frequency (screened) $\cong$ 1.2 eV (EELS)	low-density of charge carriers	OK
special space groups in diffraction patterns	curved space description?	OK
specific heat measurements are inconsistent with 2D behaviour	the HTSM phenomenon is three-dimensional	OK

(Notations: SC - superconductor, RE - rare-earth element)

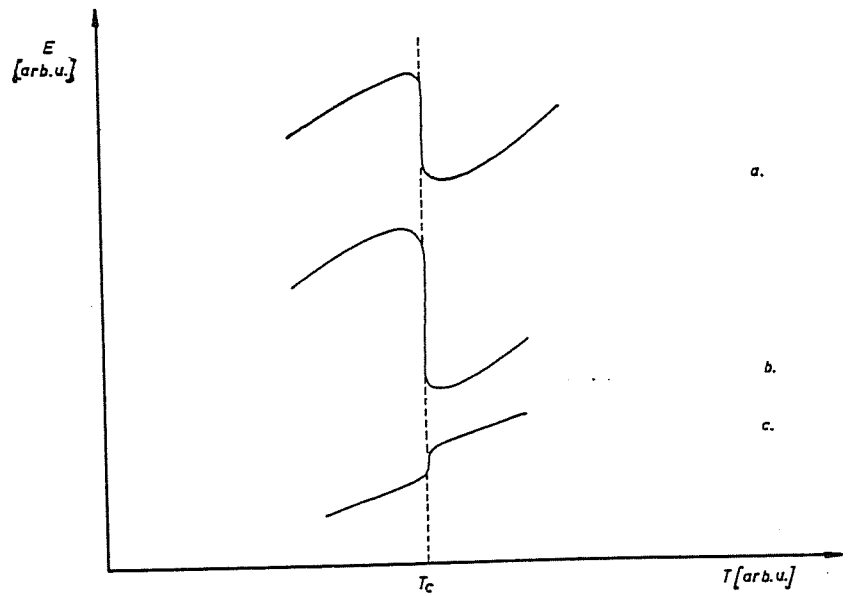


Fig.1. A schematic diagram of a phase change and the idea of electronic stabilization.

a. total energy

b. structural energy

c. electronic energy

(For the clarity a phase transition of the first kind is given.)

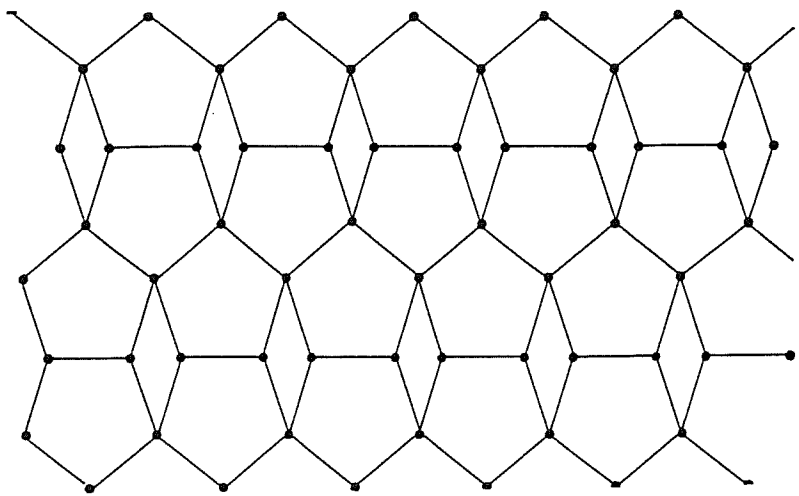


Fig.2. A tessellation of the 2D plain sheet by regular pentagons and rhombuses.

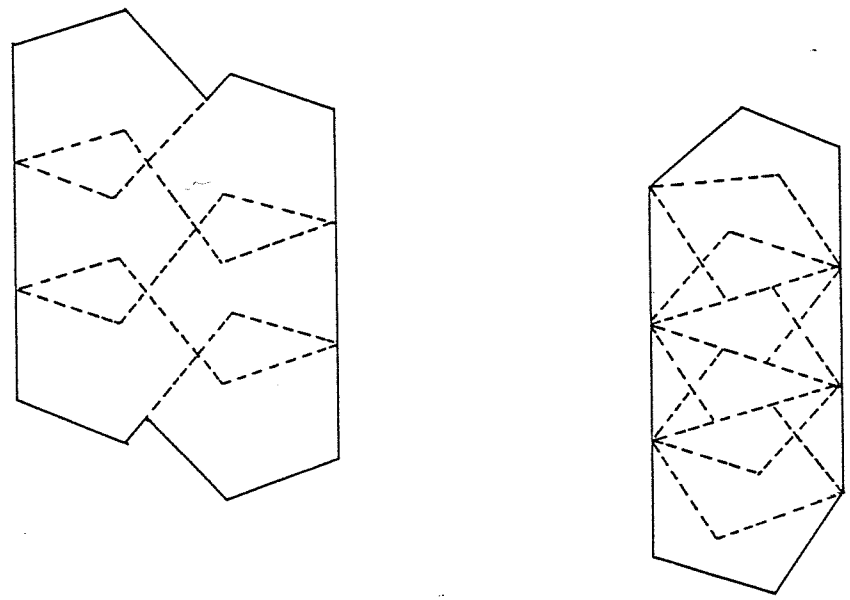


Fig.3. The example of the possible overlapping tessellations of regular pentagons in 2D.

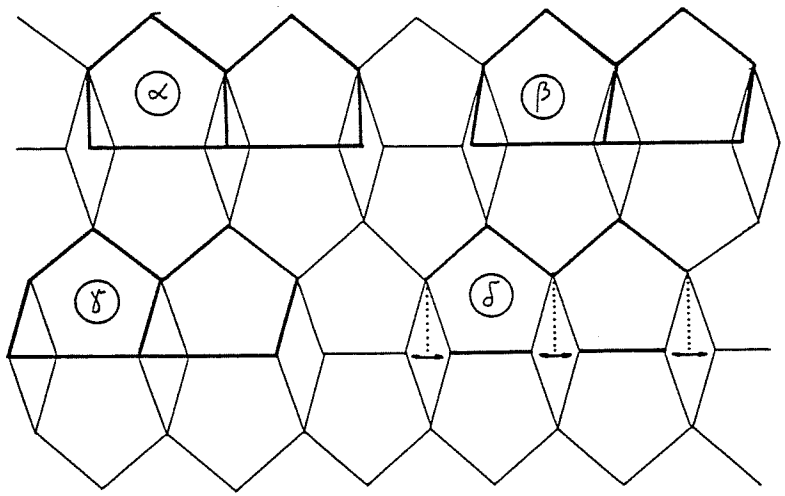


Fig.4. Satisfying the LRO requirements by the non-regular pentagons, (α, β, γ and δ are shown as examples).

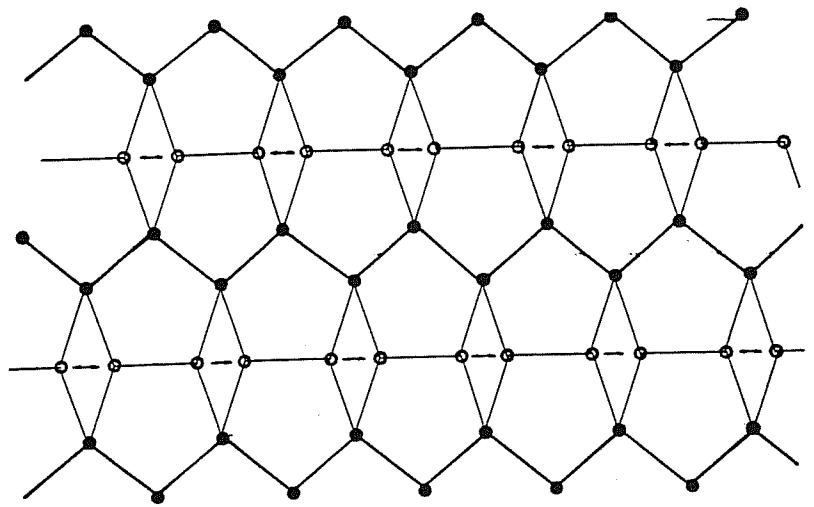


Fig.5. A dynamic solution of the geometric frustration in 2D. (N.B.: Rigid zig-zags and soft fence chains are altering.)

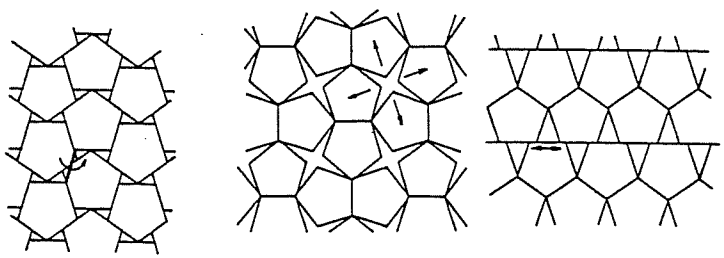


Fig.6. The different type of tailing by regular pentagons. (The frustration is indicated by arrows.)

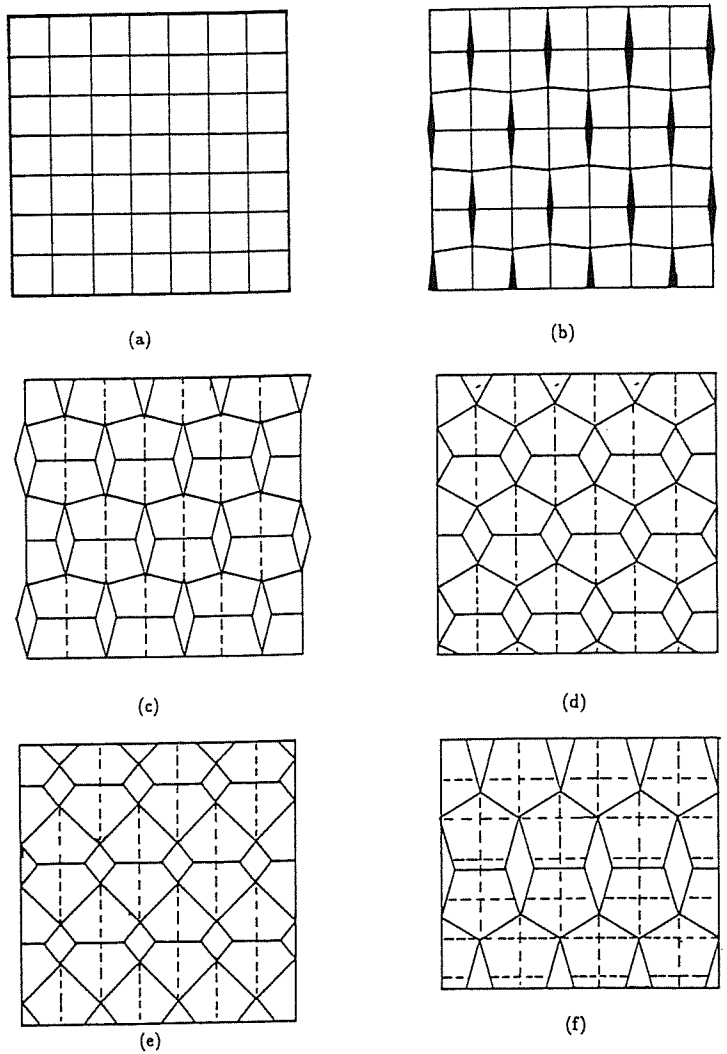
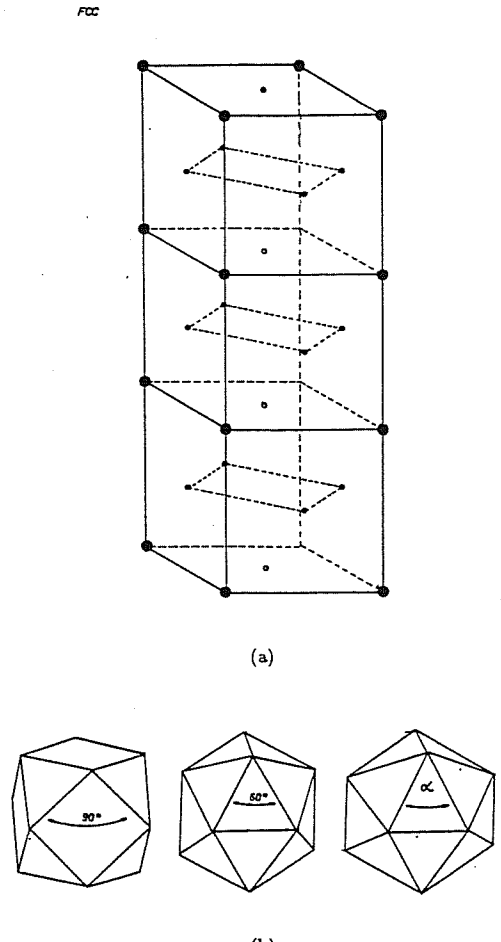


Fig.7. A continuous transformation from a square lattice to pentagonal tessellation. The different stages are given. For regular pentagons a shrinking and expansion in perpendicular directions have to be introduced. (Starting from square-lattice (a.) is presented the transformation through different stages (b.,c.,d. and e.). The expansion is shown too, (f.).)



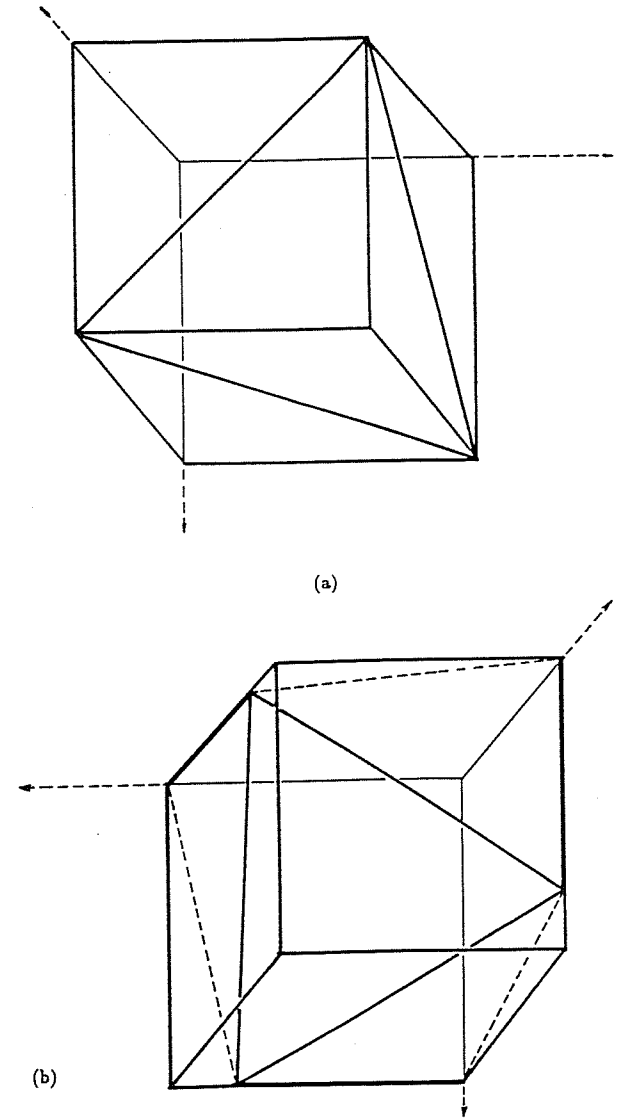
(a)

(b)

Fig.8. The transformation of FCC Wigner-Seitz cell into an ICP arrangement.

a. An FCC 'tower' (N.B. The perpendicularly twisted squares are well observable for the construction of the Wigner-Seitz cell.)

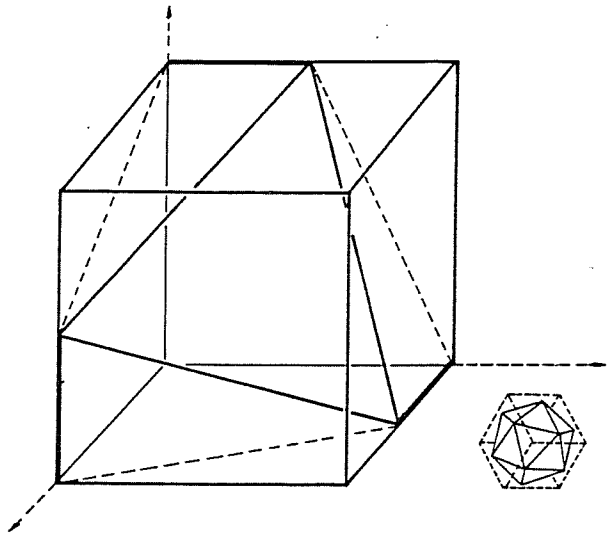
b. Deformation of the FCC Wigner-Seitz cell into icosahedra and deformed icosahedra.



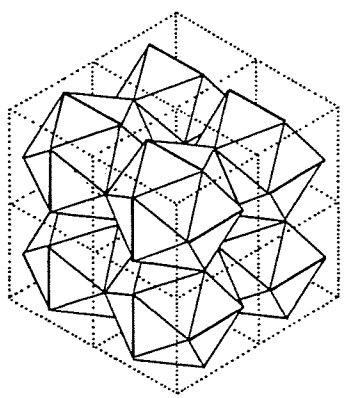
(a)

(b)

Fig. 9



(c)



(d)

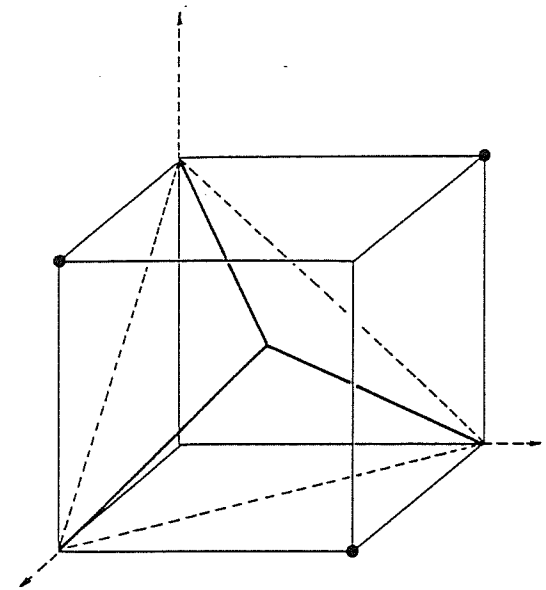
Fig. 9. A characteristic part (1/8) of the elementary cell and its transformation by tilting.

a. the 1/8 FCC elementary cell,

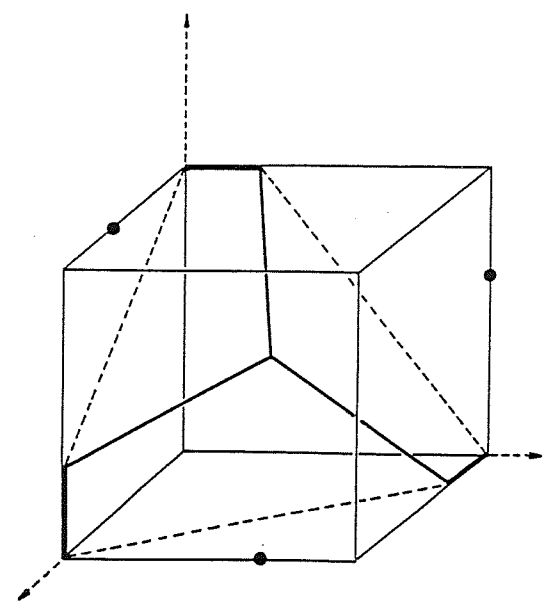
b. deformation by tilting, seeking to icosahedron (1/8),

c. 1/8 icosahedron, the whole arrangement in insert,

d. a group of icosahedra.

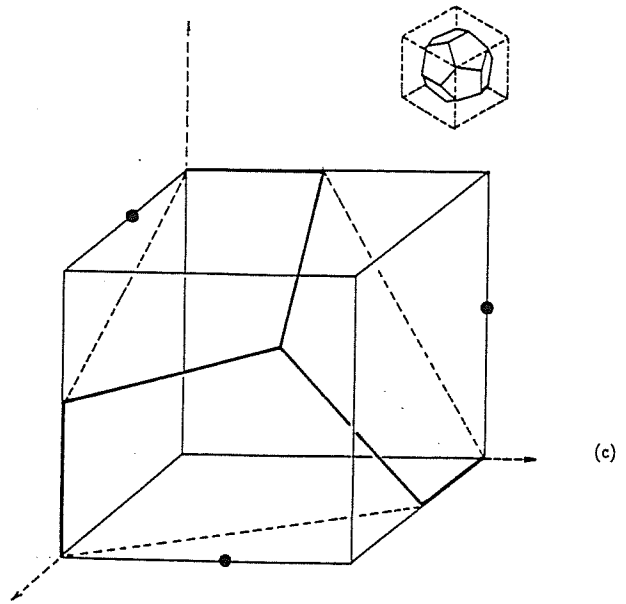


(a)

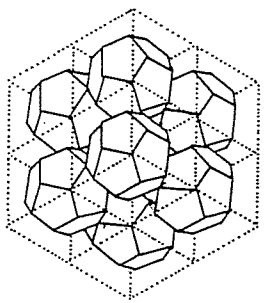


(b)

Fig. 10



(c)



(d)

Fig.10. A characteristic part (1/8) of the Wigner-Seitz cell (the geometric dual of the elementary cell) and its continous transformation by tilting.

a. the 1/8 FCC Wigner-Seitz cell, (the atomic positions are displayed too),

b. a deformed stage, seeking to dodecahedron,

c. a 1/8 dodecahedron, the whole arrangement is displayed in insert,

d. a group of dodecahedra.

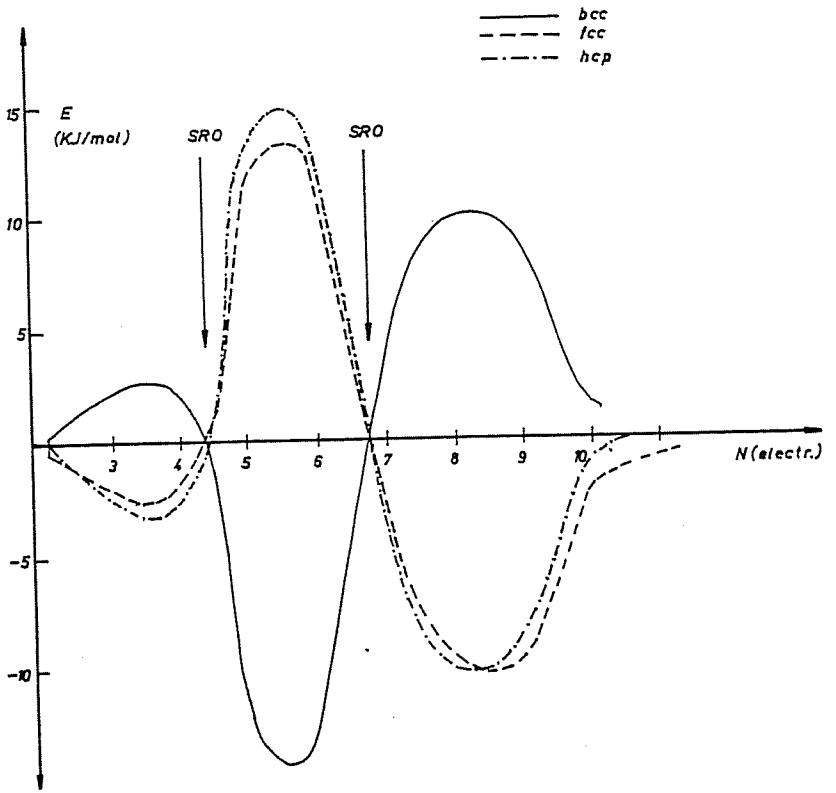
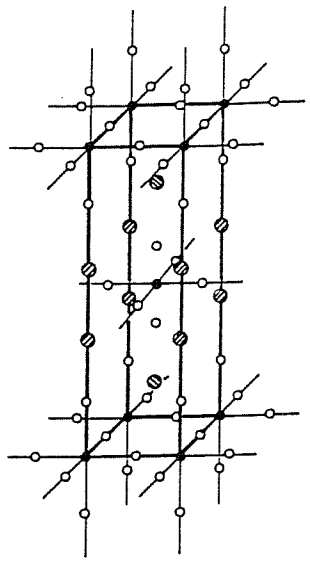


Fig.11. Calculated [72] preferable LRO and SRO intervals against the free electronic number (N) in alloys. The SRO preference is indicated by arrows.

(a)



(b)

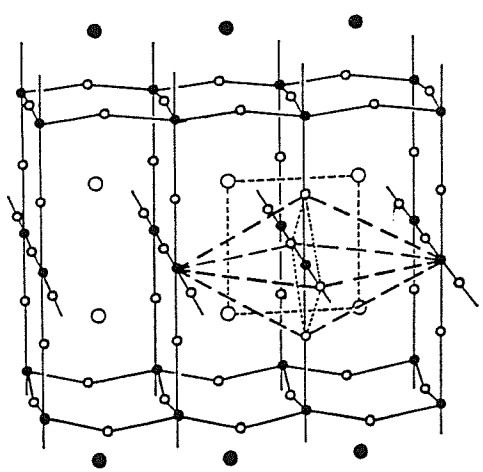
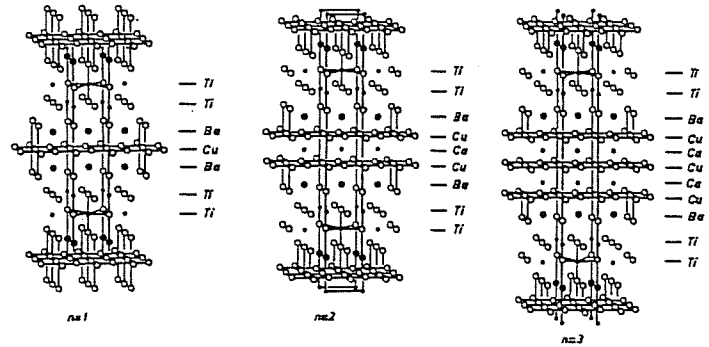
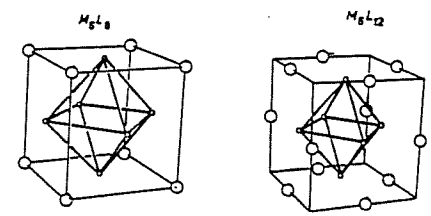


Fig. 12



(c)



(d)

Fig.12. Examples of the Frank-Kasper clusters in HTSM-s:

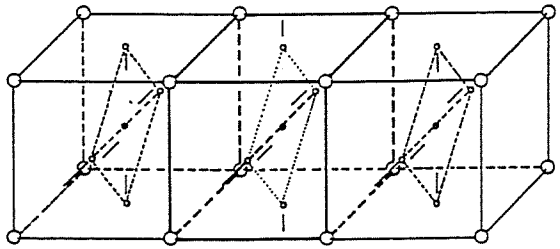
a. $La_{2-x}Sr_xCuO_4$ (for example: around Cu atoms, denoted by ●)

b. $Y_1Ba_2Cu_3O_{7-z}$ (for example: around Cu atoms in chains, denoted by ●),

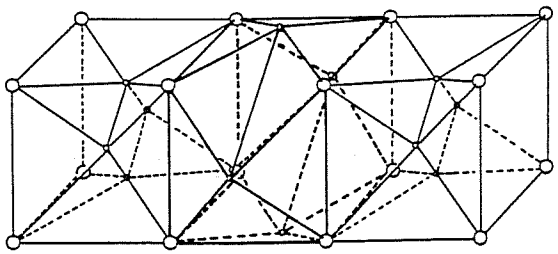
c. Aurvillius phases (for example: around Cu atoms, denoted by ●)

d. Cheverels (for examle: around M atoms in M_6L_8 and around L atoms in M_6L_{12}).

(N.B. The perpendicularly twisted squares are well observable.)



(a)



(b)

(c)

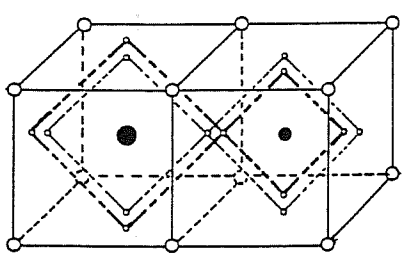
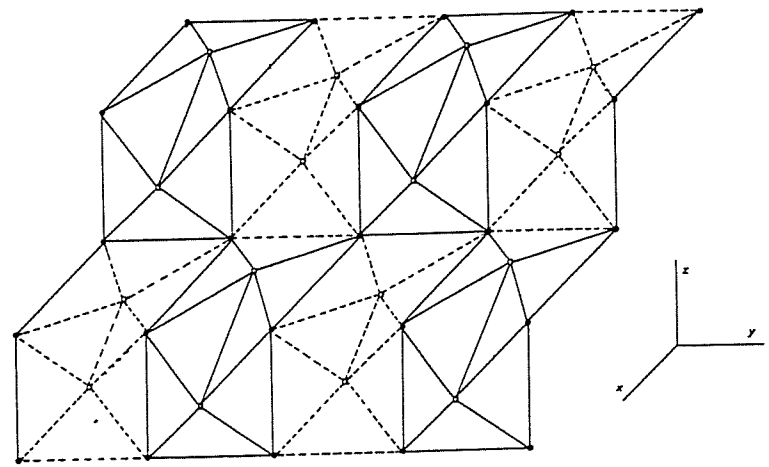


Fig. 13



(d)

Fig.13. The collective frustration mechanism in HTSM

a. the non-fluctuated picture (the breathing of oxygen neighbourhood is denoted by arrows)

b. the responsible coordination spheres and the dynamic frustration (sliding wave). The central Cu-atoms are not displayed for clarity.)

c. frustration in perpendicular sheet,

d. a sliding wave arising from frustration.

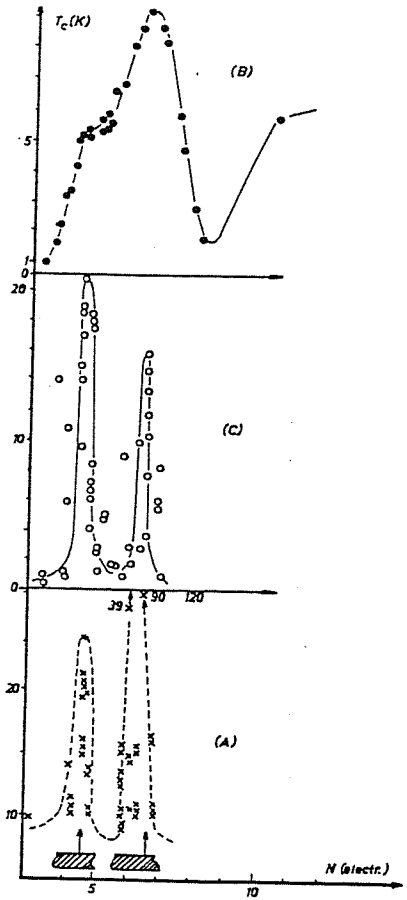


Fig.14. T_c of various superconductors versus the electronic concentration (e/a). For the clarity the SRO preference (as in Fig.11.), is also indicated by shadowed area indicated by arrows.

a. high T_c ceramics and some other compounds, (the highest T_c-s are denoted by arrows only)

b. amorphous alloys,

c. alloys with A 15 structure.

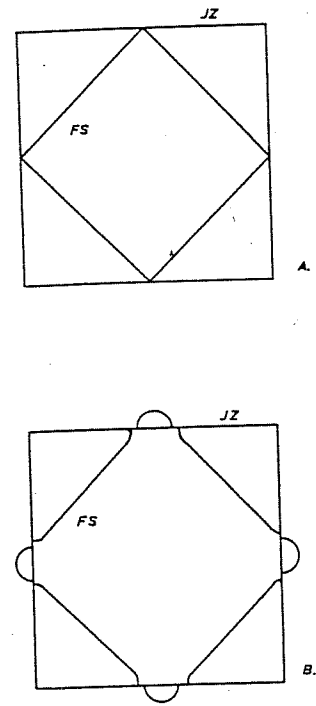


Fig.15. A schematic diagram of FS nesting in JZ in 2D.

a. full nesting (nonmetallic, stable)

b. tuned away from nesting (unstable, seeking to stable nesting in clusters)

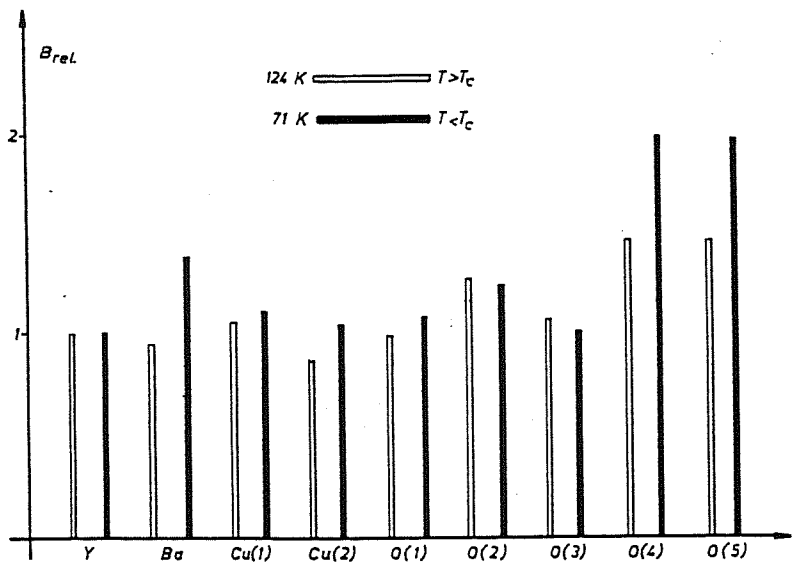


Fig.16. Relative to Y Debye-Waller factors (B_{rel}) in $Y_1Ba_2Cu_3O_{7-\delta}$ ceramics in orthorombic phase (T_c = 92.5 K).

a. above T_c (T = 124 K; $\Delta T/T_c$ = 0.34)

b. below T_c (T = 71 K; $\Delta T/T_c$ = -0.23)

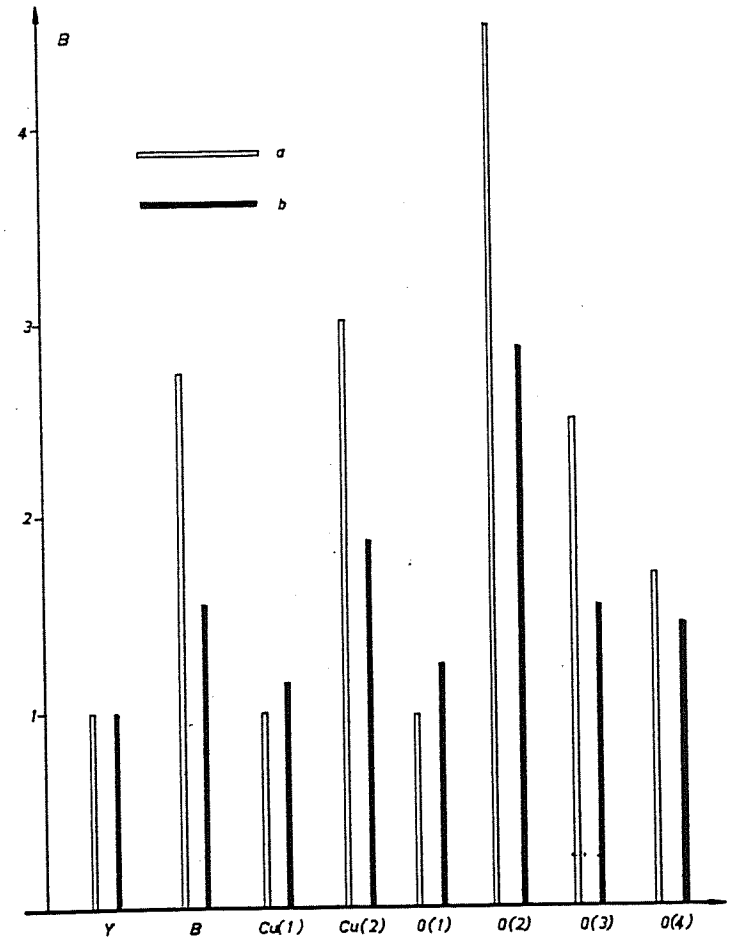


Fig.17. Change of the relative DW factor (B), (normalised to Y) of $Y_1Ba_2Cu_3O_{7-\delta}$ irradiated by fast neutrons.

a. before irradiation (T_c = 91 K)

b. after irradiation (T_c = 89 K)

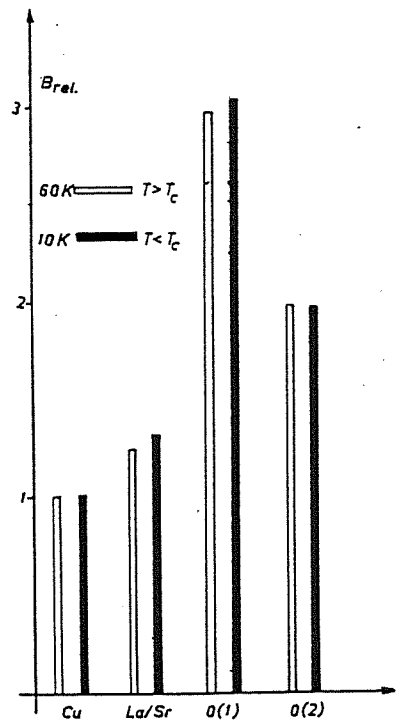


Fig.18. Relative Debye-Waller factor (B_{rel}) to Cu in $La_{1.85}Sr_{0.15}CuO_4$ superconductor in the same orthorhombic phase (T_c = 37.5 K)

a. above T_c (T = 60 K; $\Delta T/T_c$ = 0.60)

b. below T_c (T = 10 K; $\Delta T/T_c$ = -0.73)

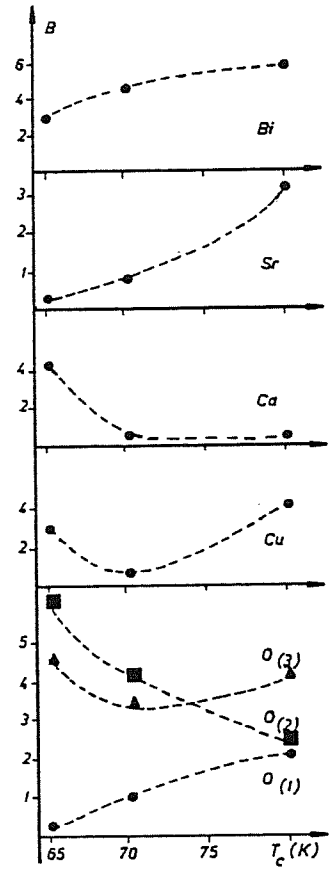


Fig.19. Comparison of DW-factors (B) versus different T_c-s for compounds:

$Bi_1Sr_2Ca_1Cu_2O_{8-\delta}$ (T_c = 81 K)

$Bi_2Sr_1Ca_2Cu_2O_{8-\delta}$ (T_c = 70 K)

$Bi_2Ca_{1.5}Y_{0.5}Sr_1Cu_2O_{8-\delta}$ (T_c = 65 K)

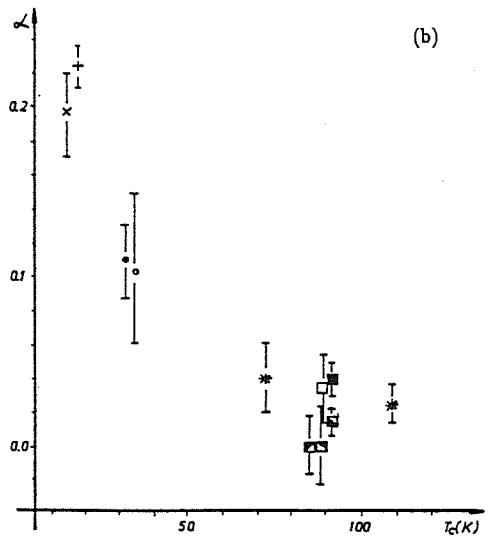


Fig.21. The isotope effect ($T_c \propto M^{-\alpha}$) of HTSM

× Ba-Pb-Bi-O [140]

\+ Ba-Pb-Bi-O [141]

O La-Sr-Cu-O [142]

. La-Sr-Cu-O [143]

□ Y-Ba-Cu-O [144]

■ Y-Ba-Cu-O [145]

□ Y-Ba-Cu-O [146]

□ Y-Ba-Cu-O [147]

□ Y-Ba-Cu-O [148]

* Bi-Sr-Ca-Cu-O [149]

a. ΔT_c versus T_c,

b. α versus T_c

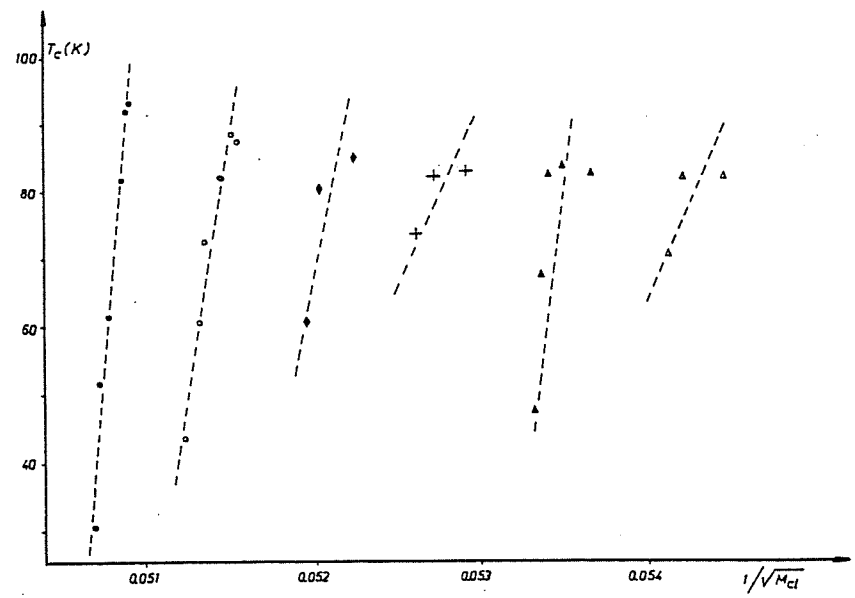


Fig.22. T_c versus reciprocal square-root of frustrated cluster masses ($Ba_{2-z-y}La_yCa_zCu_1O_{2+x}$) in Y-Ba-Cu-O type ceramics. Grouping by the z-parameter:

● z = 0

○ z = 0.1

◆ z = 0.2

\+ z = 0.3

Δ z = 0.4

▲ z = 0.5

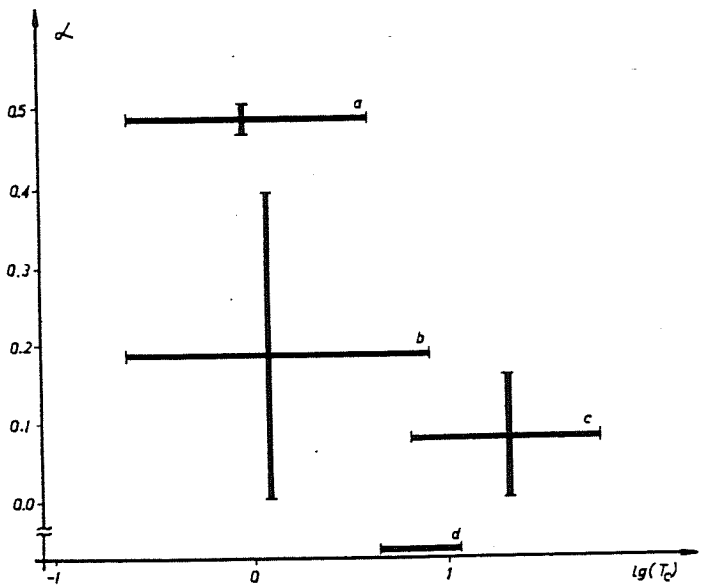


Fig.20. Range of exponents of the isotope effect ($T_c \propto M^{-\alpha}$) against the logarithm of T_c-s [18].

a. simple metals

b. transition metals and alloys

c. HTSM

d. Palladium hydride

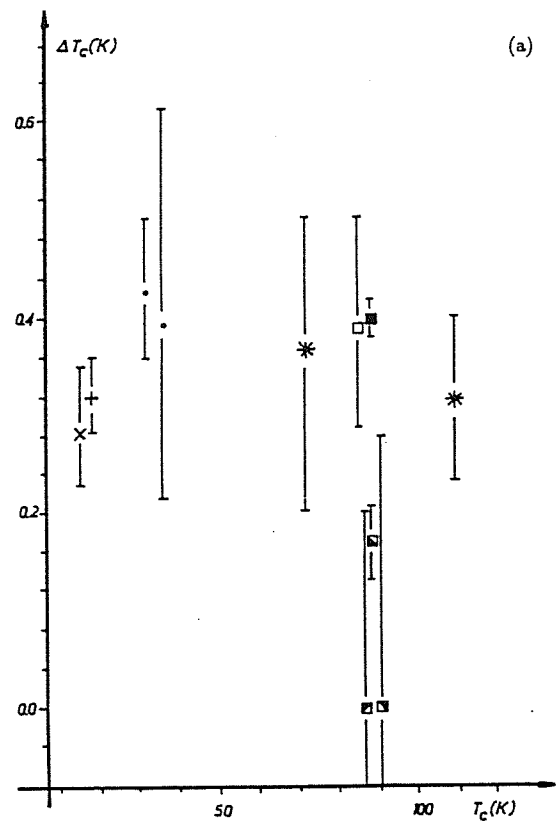


Fig. 21

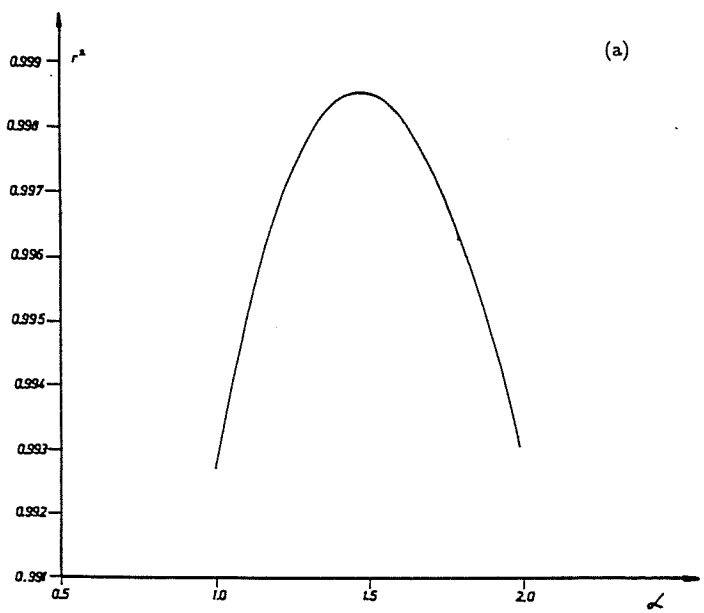


Fig. 25

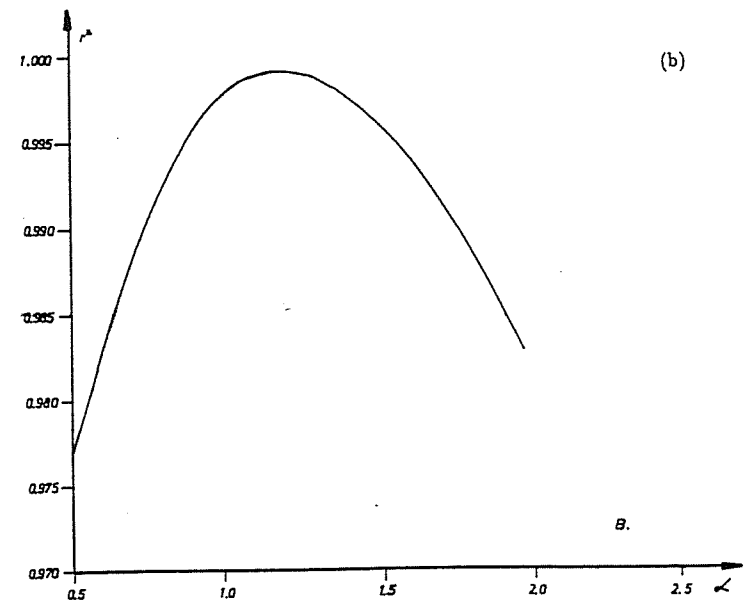


Fig.25. Choice of the best fit for the mass-exponent (α') versus standard deviation of regression:

a. for Bi-layers,

b. for Pb-layers.

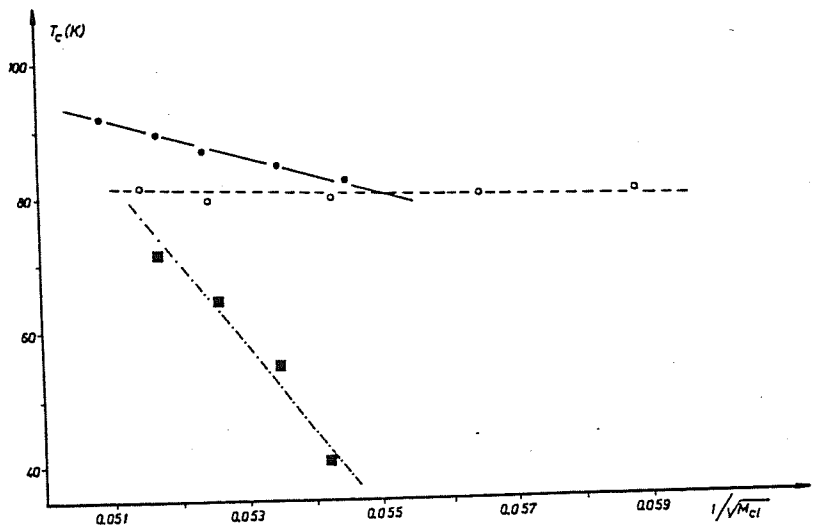


Fig.23. T_c dependence against $M_{cl}^{-0.5}$ in compounds:

a.○ $La_1Ba_{2-2y}Ca_{2y}Cu_3O_{6+x}$

b.● $Y_1Ba_{2-2y}Sr_{2y}Cu_3O_{6+x}$

c.○ $La_1Ba_{2-2y}Sr_{2y}Cu_3O_{6+x}$

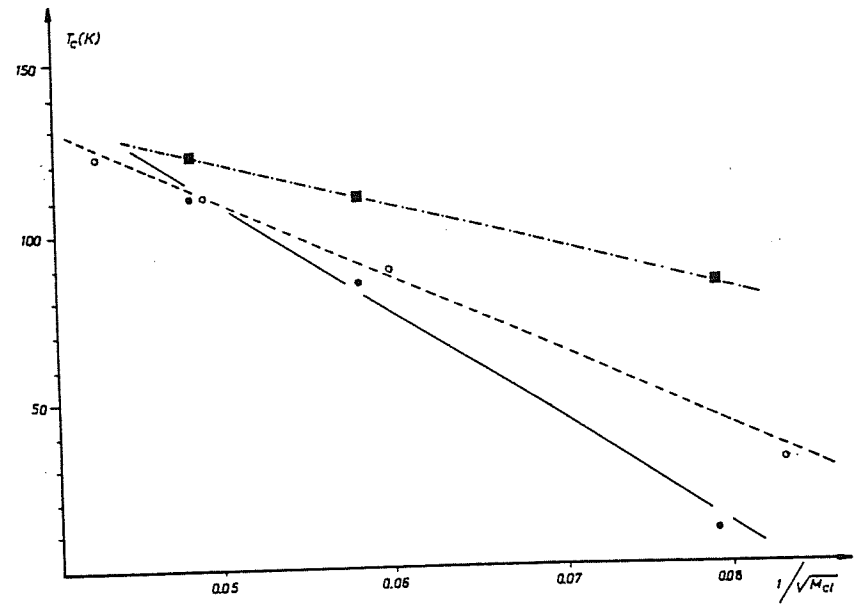


Fig.24. T_c dependence against $M_{cl}^{-0.5}$ in compounds:

a.■ $Tl_2Ba_2Ca_xCu_yO_z$

(x=0,1,2; y=1,2,3; z=6,8,10)

b.○ $Tl_1Ba_2Ca_xCu_yO_z$

(x=0,1,2,3; y=1,2,3,4; z=5,7,9,11)

c.● $Bi_2Sr_2Ca_xCu_yO_z$

(x=0,1,2; y=1,2,3; z=6,8,10)